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An integrated "process modelling-life cycle assessment" tool for the assessment and design of water treatment processes

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Abstract
Purpose The application of Life Cycle Assessment (LCA) to the design of water treatment plants is hampered by: (1) a large diversity of unit processes, (2) the high variability of the operation conditions in relation with the water quality input, and (3) the range of possible technical solutions to fulfil the treatment needs. For a consistent prospective assessment, the LCA should be based on the simulated functioning of the unit processes rather than on average data, as it is most often the case when no real data are available. Here, a novel, integrated and flexible process modelling-life cycle assessment (PM-LCA) tool for design and LCA of water treatment technologies is presented.
Methods The tool (EVALEAU) was developed in Umberto® (v5.5) using the Python language for code scripting. A library of unit process (UP) modules was built. Each module is a detailed and highly parameterized model of a specific water treatment process, which is further linked with the software PHREEQC® for water chemistry calculation. Input data are: water composition, design, operation parameters, including literature or user-defined values. The modules are linked to Ecoinvent datasets (v2.2) for background processes. By combining the modules, water treatment chains can be designed and evaluated in Umberto® with a high level of detail and specifications. A sensitivity analysis toolbox (Morris method) was included for the identification of the process parameters mainly affecting the impact results.
Results and discussion The tool was successfully applied to the test bed case of an existing drinking water plant located in the Paris region. The conventional LCA results, based on average recorded data, were compared with the results obtained using the PM-LCA tool. Modelling results for technical parameters were also compared with data collected on site. An overall good agreement between simulations and real data was obtained, proving the relevance of the developed tool. Sensitivity analysis indicated that ozone production and transfer into water are the main technological parameters influencing climate change (taken as example since it is of high interest for stakeholders), which have therefore to be fine-tuned.
Conclusions The EVALEAU tool successfully solves the challenge of linking LCA results to the related engineering design choices, from the assessment and eco-design perspectives. The concepts and methodologies embedded within the tool provide the user with complementary views of the designed system, in terms of potable water quality, design and operation parameters and environmental impacts generated over its life cycle.

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1 Introduction

Nowadays, Life Cycle Assessment (LCA) methodology is increasingly used to evaluate the environmental performances of processes, products and services and potentially represents a powerful tool for eco-design. As suggested by Azapagic and Clift (1999) and Azapagic et al. (2006), the integration of environmental criteria through LCA for instance, at the very early stages of process design is essential in the life cycle optimization of the designed system, focusing both on the foreground and background processes. Nevertheless, it still needs the development of adapted integrative methods and tools.

Indeed, life cycle inventories are traditionally based on average data (material and energy inputs and outputs) collected on site or estimated from literature or from modelling studies performed prior to the LCA study. This approach has recognized shortcomings when applied on processes characterized by highly variable design and operation parameters. This is the case of pollution treatment technologies, e.g., water treatment, which are composed of a chain of unit processes (UP) linked together by the functional unit (the water flow to be treated). Raw water undergoes subsequent quality changes across the chain of UPs, until the targeted output quality is reached. Water treatment technologies are characterized by: (1) different types of raw water treated (sea, rivers, groundwater, specific effluents, sewage, etc.) and the variability of their properties (local composition variations, flow rates, seasonal or other time related constraints, etc.), making each treatment plant unique and site specific; (2) highly adaptable operation conditions in response to the raw water quality fluctuations (variation of energy and material input/output); (3) many possible technical solutions (i.e., types of UPs and their combinations) in the design phase; (4) variability of UP's operating conditions (physico-chemical parameters) which are most often chosen based on economic considerations. Because for most UPs there are only limited Life Cycle Inventory (LCI) data available, currently it is not possible to set up databases considering points (1) to (4). As a result, the application of LCA to water treatment is hampered and in most of the cases the LCA results are not relevant for the comparison of different technologies or for the identification of environmental hot spots.

The water quality and the operation parameters determine the required energy and material consumptions. Therefore, the LCI is dependent on the technological specifications and project constraints. Consequently, the building of a highly parameterized LCI is mandatory to properly evaluate the environmental impacts of water treatment chains. Moreover, the use of LCA as a tool for eco-design requires a predictive and prospective LCI, which has to take into account the elements of points (1) to (4).

In the past decade, significant efforts have been made in order to cope with the challenge of integrating environmental criteria into the design of process-based plants. Sugiyama et al. (2008) suggested a framework for decision-making support on process design, integrating technical, economic and environmental aspects and a similar approach was proposed by Khan et al. (2001). However, the application of these concepts in the industrial practice remains difficult and process design is often considered as a preliminary step to LCA instead of being fully integrated in a coherent framework (Bojarski et al. 2008; Iosif et al. 2010; Kniel et al. 1996; Vince et al. 2008). The indirect environmental impacts due to off-site pollutant emissions of background processes were taken into consideration by Bernier et al. (2011) by linking a power plant model with Ecoinvent-like modules, corresponding to the background processes involved. Chen et al. (2004) went a step further and proposed a fully integrated framework linking the ASPEN software for process modelling and Excel to carry out the LCA, with applications to the chemical industry. The automated connection between those tools and databases makes it possible to get the different results in parallel and not consequently, proving a better understanding of the design alternatives on the LCA results. Nevertheless, the approach of Chen et al. (2004) cannot be applied to all types of industrial processes, as for example the depollution technologies, because of the lack of appropriate modelling tools. Concerning conventional LCA studies (based on site inventories) on potable water production, a state of the art was presented recently (Igos et al. 2012) and therefore this subject is not detailed here. The most of the available studies focused on membrane technologies for desalination and very few approached the conventional processes (Vince et al. 2008; Raluy et al. 2005; Friedrich 2002; Sombekke et al. 1997).

A certain number of exposed bottlenecks have been successfully solved through the development of a fully integrated process modelling-life cycle assessment (PM-LCA) tool for water treatment technologies. The tool named EVALEAU fulfils two functions: *process modelling–design aid* and *environmental diagnosis*.

In this paper, the principles and methods used to develop the tool are described, then its validation is presented and discussed through a test bed case.

2 Methods

2.1 EVALEAU tool development

The developed PM-LCA tool, hereafter named EVALEAU, is aimed at covering the specificities of water treatment technologies and has to fulfil at a minimum the following

requirements: (1) calculate the LCA results of different water treatment (foreground) processes according to the ISO 14040-44 standards, using conventional LCI databases for the background processes and recognized LCIA methods; (2) allow easy combination of UPs in different treatment chains, in order to assess a variety of different technologies; (3) account for the influence of design and operation parameters on the foreground LCI; (4) allow easy modification of the default values of process parameters (user-defined values) for calculating the corresponding LCI in order to evaluate the LCA results for different working conditions of the plant; and (5) automatically identify the hot spots, i.e., the process parameters having the major influence on LCA results.

In order to fulfil the first requirement, the software Umberto® v5.5 (http://www.ifu.com/en) has been chosen as working environment because of its capability to resolve complex flow networks. The inventory modules are uploaded from LCI database Ecoinvent (Weidema et al. 2009), for energy suppliers, chemicals, transports, etc., or are defined by the user through specific scripts, for the specific UPs of water treatment. The integrated scripting capability of Umberto® was exploited to create a complementary library of independent modules dedicated to the different UPs of water treatment technologies, which allowed complying with the second requirement. The library allows building the foreground process chain (i.e., EVALEAU modules for the water treatment chain) which is further linked to the required background processes (i.e., Ecoinvent modules for electricity and chemicals production). The principle of the developed tool and of the LCI calculation is schematized in Fig. 1.

The modules stored in the EVALEAU library are parameterized models, written in Python™, which calculate chemicals and energy consumptions and substance emissions at the level of each UP. In addition, each UP model provides the technical design and operation data necessary to link the UPs in the whole process network and to assess the process efficiency. The Water Quality Data (WQD) is a set of 168 criteria including generic parameters (temperature, pH, turbidity, etc.), organic matter parameters (UV absorbance, dissolved organic carbon, etc.), pathogenic microorganisms, inorganic compounds, micro-pollutants, reaction products. The WQD template is stored in an Excel file, directly available (reading and writing) to the Python™ scripts and has to be fed by the user with specific data concerning the raw water of the case under study. A sensitivity analysis tool relative to the model parameters was implemented as well in order to fulfil the fifth requirement.

In the Umberto environment (see Fig. 1), the UP modules are first linked each other to build the water treatment chain (foreground level) and then linked to the appropriate Ecoinvent (currently used database) background modules. At the level of a UP module, the input data are: (1) water quality data, being issued from the raw WQD file or calculated by the previous module, (2) specific parameters of the process (user values or default values). This model architecture ensures specific inventory calculation at the level of each UP, of the complete plant and of the plant's life cycle, thus satisfying the third requirement.

Besides the LCI, the UP models calculate engineering design data as well — a brief overview of the UP design and its overall efficiency, which are mandatory from an ecodesign perspective (e.g., electric power to be installed, water velocity in pipes). They are currently stored in an automatically created spreadsheet (engineering design data report), together with the intermediary and output WQD. The results obtained from the tool are as follows: (1) energy and chemicals consumptions at

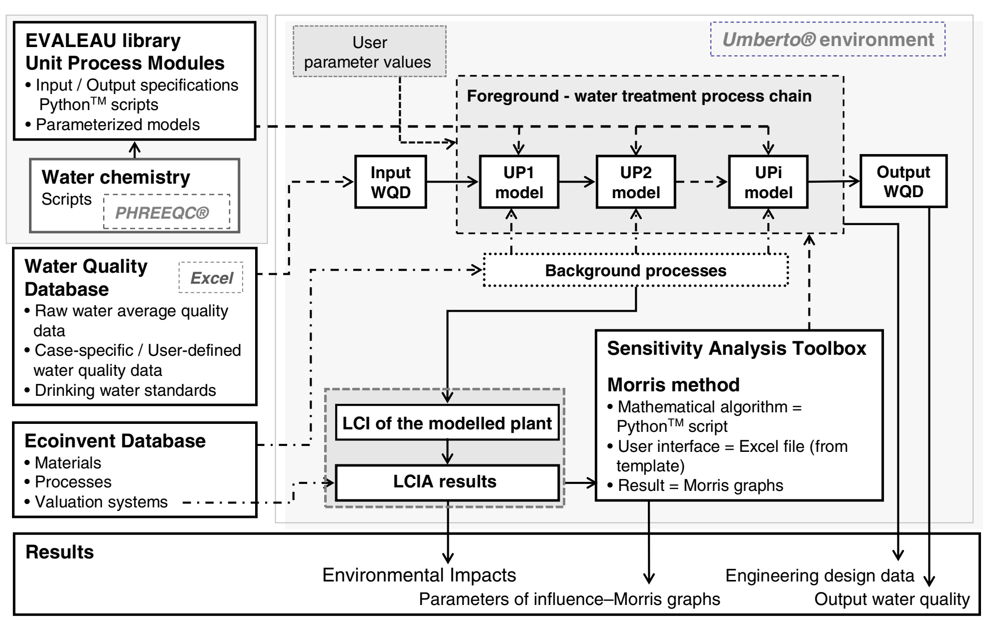

Fig. 1 Principle of the EVALEAU tool — automatic linkages between different software tools, main tasks and results

the level of each UP and complete LCI, (2) LCIA results, (3) output water quality, (4) engineering design data, and (5) sensitivity analysis results.

To sum up, EVALEAU is a PM-LCA tool. Its main components are the computational library of UP models, the sensitivity analysis toolbox, a set of water quality data (WQD), output spreadsheet data (WQD), engineering design report and their linkages. It fully benefits from Umberto environment and capabilities. It allows flowchart building for any water treatment plant and calculation of material and energy input/output at plant (*process modelling* function). It performs *environmental diagnosis* of the modelled plant.

2.1.1 UP modelling and parameterization

The UPs are traversed by the water flow which undergoes changes at the level of each UP. At the level of a given UP, the pollutant abatement is achieved by chemical reactions (e.g., precipitation, coagulation, oxidation) and/or separation processes (settling, filtration, etc.). The water quality can also be corrected by adding specific substances for mineralization, softening, etc. All these processes have to be characterized using chemical reaction and/or separation efficiency models. Chemicals and energy consumption in the water treatment processes is a function of the input water quality (i.e., the nature and quantity of pollutants) and of the treatment performance objective (output water quality). A literature review of existing models for water treatment processes has been carried out in order to select the best available UP models. The selected models are reference models in their respective domain and have been developed by recognized scientific organization (e.g., the WTP modelling approach developed by the US EPA for assessing Disinfection By-Products formation; WTP manual 2001). An additional selection criterion was the good agreement of the models with industrial practices.

The models consist mainly of a set of equations defining energy and mass balances, for steady state functioning conditions. The efficiency of separation operations and kinetic performances were used for each type of UP and related equipment (e.g., a given type of settler, filter), using literature and constructor specifications as default values.

In order to model the chemical reactions in aqueous solutions the geochemistry software PHREEQC® (Parkhurst and Appelo 1995) was used, because of the completeness of water chemistry models and databases included, and of its wide scientific recognition. A library of PHREEQC scripts for each UP was built, to be used by the corresponding Python script. Concerning the microbiology, results of the European project Microrisk (Smeets et al. 2006) were used in terms of mean elimination capacity of pathogen per UP. For the disinfection UP, conventional models were used combining hydrodynamics and imposed residual dose of oxidant.

The flexibility of the tool is ensured by the high parameterization of the UP models. The adjustable process parameters are a set of data that define: engineering design choices (e.g., pipe diameter, pump efficiency, device hydrodynamics), technical and productivity constraints (e.g., height to be pumped, filter area and backwashing schedule), and legal constraints (e.g., CT=(contact time) × (residual oxidant concentration), which is a disinfection requirement criterion) or pollutant abatement requirements.

The models stored in the EVALEAU library are generic and their parameters are set to default values, collected from literature, guidelines or expert recommendations. They are representative of hypothetical average working conditions of the unit processes. Defining the parameter values enables the user to modify the generic version of the model and to get a very specific model, more representative of the case under study. The comprehensive parameterization of the UP models allows users to adapt to specific situations, which is a key feature of EVALEAU tool. The modelling strategy used allows therefore fulfilling the fourth and fifth tool requirements.

2.1.2 Sensitivity analysis

The highly parameterized modelling approach generates LCI results for a high number of parameter datasets (about 100 for a conventional plant model). As a result, it is very difficult to assess their influence on the results, and to identify the engineering design and operation choices which mostly affect the LCIA results per impact category. This shortcoming was resolved by integrating sensitivity analysis relative to the model parameters, using the Morris approach (Morris 1991; Campolongo et al. 2007).

In the Morris method, model parameters but also input variables can be considered. They are both referred as factors and k is their number. The space of factors is discretized in p levels; each factor varies over the p levels. The variation of the model result due to the variation of one factor is called an elementary effect (EE) (derivative-based approach). The variation of one factor is realised as follows. The first point is randomly determined. Then, the factor value is switched to a different level, which creates a trajectory of $(k+1)$ points in the k-dimensional parameters' space. Thus one trajectory allows calculating one EE for each factor. The Morris method consists in generating r trajectories and running the corresponding model calculations. It is then possible to calculate r EEs for each factor. The procedure is repeated for each factor. In the basic version of the Morris method, the mean of the EEs and the standard deviation are computed for each factor and used as sensitivity measures to evaluate the factors' influence on the model.

This method was selected since it is easily understandable, it has low computational costs and it works almost on every kind of model. The method provides a graph which

can be interpreted without considering the details of the mathematical method. Each model parameter is represented by a point and, depending on its position on the graph; qualitative information about the parameter influence can be deduced. The more a parameter is influent, the more its position will be on the right of the graph. The less linear is the parameter's influence, the higher the point will be on the graph. The sensitivity analysis points out the key parameters to be further studied for eco-design.

2.2 Test bed case

The case study of a drinking water production plant, situated on the Seine river in the Paris region, has been used to prove the reliability of the tool while illustrating the concepts and methods implemented. The treatment chain is quite representative of conventional drinking water production and is composed of the following operations (Fig. 2): pumping, pre-ozonation, coagulation/flocculation/settling, clarification by biolite filtration, inter-ozonation, granular activated carbon (GAC) filtration and disinfection by chlorine.

First, average site data from yearly recordings were used to carry out a conventional LCA (see Igos et al. 2012, for a detailed discussion of the LCA results). The site inventory reference year is 2007, the average production rate during the reference year was 1,525 m^3/h. The available site data include: electricity consumption for the whole plant, quantities of purchased reactants and GAC. So, the LCI of the plant is based on total yearly consumptions, specific detailed electricity/reactants consumption by unit process being not available.

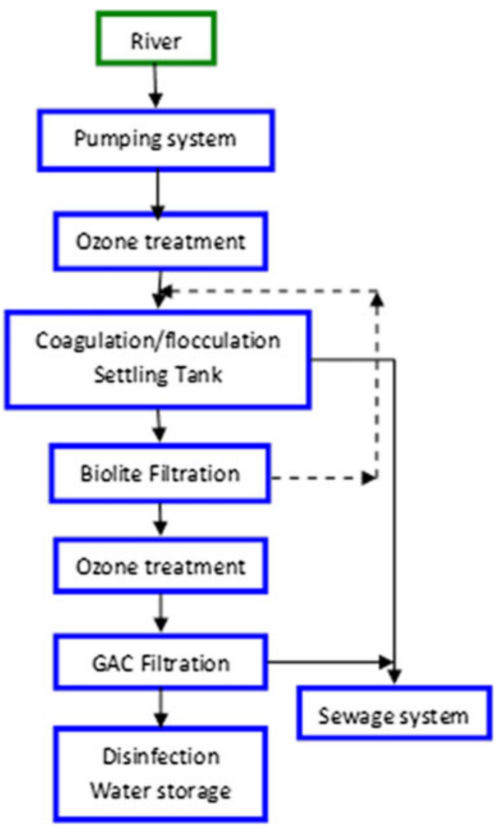

Fig. 2 Flowchart of the studied plant

Second, process modelling was coupled with the LCA approach within the EVALEAU tool. This approach allows representing the plant's flowsheet as it actually is: the chain of UPs is simulated using the respective modules from the EVALEAU library, further adapted to the site conditions, as explained in the following. The ozonation operations use air as feed gas for ozone production and take place in two different contactors, because of the different objectives, respectively enhancing the coagulation efficiency (pre-ozonation) and oxidizing the small organic molecules for a better adsorption in the GAC filters before disinfection. Aluminium sulphate is used as coagulant, polymers are added for flocculation. Coagulation/flocculation/settling take place in a compartmented device, equipped with scrappers. The filtration operations run by gravity in open devices, equipped with fixed beds of appropriate granular media. Backwashing is realized with water and compressed air. The biolite washing effluent is returned to the coagulation step whereas sludge from the settler and GAC washing effluent are sent to a separate treatment site. As no data were available on sludge treatment, this UP was not considered neither in the conventional LCA nor the PM-LCA, and this is a limitation of the presented case study. Model development for sludge treatment (sludge from potable water plants) is an ongoing work. The disinfection using sodium hypochlorite is the last operation realized in the stocking reservoir. There is no intermediary pumping as water flows inside the plant by gravity. In this work, the focus is on the calculation of the foreground inventory data using the EVALEAU tool, by simulating the operating conditions of the plant. The raw water quality (used at the model input) is known from mean values recorded over many years including the reference year.

For both the conventional LCA and the PM-LCA, the functional unit chosen is "1 m^3 of drinking water at plant". Water quality has been checked in the modelling scenario for ensuring that legal limits and industrial guidelines for potable water were respected. Plant construction and decommissioning are not included; they are out of the scope of the EVALEAU tool and library at the present stage of development. Tap water distribution is out of scope as well. Both the conventional LCA and the PM-LCA were carried out using Umberto® 5.5 and Ecoinvent 2.2 (using the same background processes), and relying on the Impact 2002+ methodology (Jolliet et al. 2003) for LCIA. As the background conditions are the same, any divergence between the LCA and the PM-LCA results has to be ascribed to the foreground processes.

3 Results and discussion

3.1 Test bed case for the validation of the PM-LCA tool

The foreground water treatment process has been built in Umberto by linking the appropriate UP modules loaded from the EVALEAU library and by defining appropriate values for the process parameters. All the models used are briefly described in the Electronic supplementary material (ESM) along with the respective parameters and their values (Table S1, ESM). The first result obtained from the process simulation is the water quality at the treatment chain output and at the output of the different UPs (Table 1). Only a few data obtained by site measurements are available for the UPs and concern only the major parameters that have a great importance for the evaluation of treatment efficiency, such as the UV absorbance and turbidity. It was found that the simulated values are in relatively good agreement with the measured values or with the limits imposed by the current regulations.

The estimation of the chemicals and the electricity consumptions is not straightforward due to the high variability in time of the raw water quality. A consistent estimation of these data is however mandatory. Field data for chemicals and electricity consumptions at plant are used to calculate average values over the reference year. They are compared with simulation results in Table 2. It is observed that the relative difference does not exceed 10 %, and therefore the modelling approach is considered as consistent. It is worth mentioning that the water industry know-how about consumption forecasting does not seem to provide better estimates than our modelling.

Details on plant inventory and the corresponding data sets (Ecoinvent2.2) used for background processes are presented in Table S2 (ESM). Calculated detailed inventory by UP (simulation results with EVALEAU tool) is given in Table S3 (ESM).

As the LCIA results per inventoried substance are linearly dependent to the LCI, it is expected to have similar LCIA results for the two LCA approaches. Figure 3a confirms this expectation, showing the good agreement between the LCIA results obtained from the conventional LCA and from the PM-LCA. The results were obtained using the Impact2002+/Endpoint methodology, with European normalization, as currently implemented in Umberto®5.5.

The relative difference is even lower than for the LCIs (+2.25 % for climate change, −6.01 % for ecosystem quality, −2.79 % for human health, −5.43 % for resources). The rationale is that the damage factors in LCIA are very different from one substance to another and the individual LCIA results are finally aggregated per impact category, thus reducing the discrepancies between the conventional LCA and the PM-LCA results.

Detailed LCIA results for the studied plant are not fully presented here since this is not the objective of the present work. The conventional LCA application and results for the same plant are also presented in extenso by Igos et al. (2012). The following evaluation results are presented in the ESM: detailed endpoint results for the midpoint impact categories (Fig. S2) for the whole plant life cycle; UPs' contribution analysis based on endpoint categories (Fig. S3); UPs' contribution analysis on several midpoint impact categories (calculated ad endpoint) (Fig. S4).

An analysis of the midpoint impact categories (normalized at endpoint; Humbert et al. 2005) have shown that "non-

Table 2 Summary of the measured and modelled on-site consumptions (site inventory for 1 m^3 potable water)

Inventory item	Real on-site consumption	Modelled consumption	Error (%)
Electricity (kWh/m^3)	0.896	0.824	−7.99
Polymer (g/m^3)	0.174	0.170	0.05
Sodium hypochlorite (g/m^3)	5.92	5.50	−7.06
Aluminum sulphate (g/m^3)	62.9	62.8	0.17
GAC (g/m^3)	6.00	6.59	9.80

Table 1 Measured and modelled water quality parameters

Parameter	Average measure or imposed limit	Simulation	Observations
Settled water UV absorbance (m^{-1})	3.22	3.70	Error 14.9 %
Settled water turbidity (NTU)[a]	*<2*	0.57	In the range
Biolite filtration turbidity (NTU)[a]	0.13	0.095	Error −26.9 %
Potable water pH	*6.5–8.5*	7	In the range
UV absorbance (m^{-1})	1.26 (*<1.5*)	1.31	Error 3.9 %
Turbidity (NTU)	*<0.3*	0.016	In the range
Total hardness (French degree)[a]	*15–25*	19	In the range
Al total (mg/l)	*<0.1*	0.0033	In the range
TOC (mg/l)	*<1.5*	1.2	In the range

NTU nephelometric turbidity units

– Imposed limits are written in italic

[a]1 French degree =1 part/100,000 calcium carbonate

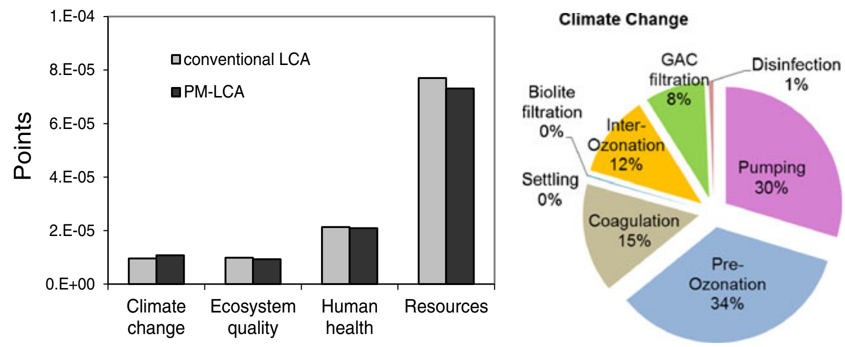

Fig. 3 LCIA results obtained from the conventional LCA and from the PM-LCA (**a**, *left*) and UP contribution to the "Climate change" impact category (**b**, *right*)

renewable energy", "respiratory effects" and "terrestrial ecotoxicity" have the most important scores within their endpoint category, "resources", "human health" and "ecosystem quality", respectively (Fig. S2). Climate change (the fourth endpoint category) is also one of the remarkable impacts. These results are explained by the fossil fuels consumption for electricity production, electricity being intensively used at plant. Fossil fuels utilisation generates the other observed major impacts: climate change, respiratory effects, ecotoxicity. The contribution analysis on all impact categories revealed similar behaviour, i.e., the dominance of ozonation processes followed by pumping and in lesser extent by coagulation operation (Figs. S2, S3 and S4). Focusing on the climate change for illustrative purpose (see Fig. 3b), the two ozonation processes are the main contributors (46 %), followed by the pumping station. This result is explained by the intensive use of electricity.

3.2 Sensitivity analysis

The Morris method implemented in EVALEAU can be applied to all the impact categories. Again, for sake of simplicity and for testing purposes, only the parameters' influence on the climate change category was analysed here and the results are presented in Fig. 4. A set of 18 parameters, with defined ranges of variations, was chosen as relevant for sensitivity analysis of the whole plant model. For example, for the ozonation operations the chosen parameters are: the ozone transfer efficiency (%), the pure oxygen fraction in the feed gas (%mol) and the ratio T10/T, which is a ratio characterizing the hydrodynamics of the device by comparing the time needed to get 10 % of a tracer out of the reactor and the theoretical hydraulic residence time.

The variation of a result due to the variation of one parameter at a time is called elementary effect (EE on the Morris graph). The mean of the EEs is represented on the abscissa and the variance on the ordinate. An influent parameter will lead to a high EE's mean, while a nonlinear influent parameter will lead to a high EE's variance. The Morris graph resulting from sensitivity analysis applied to the water treatment plant identified two main parameters, relative to the two ozonation processes (PO for pre-ozonation, IO for inter-ozonation): the ozone transfer efficiency ("OT_NU") into the contact reactors and the proportion of oxygen in the gas used for the ozone

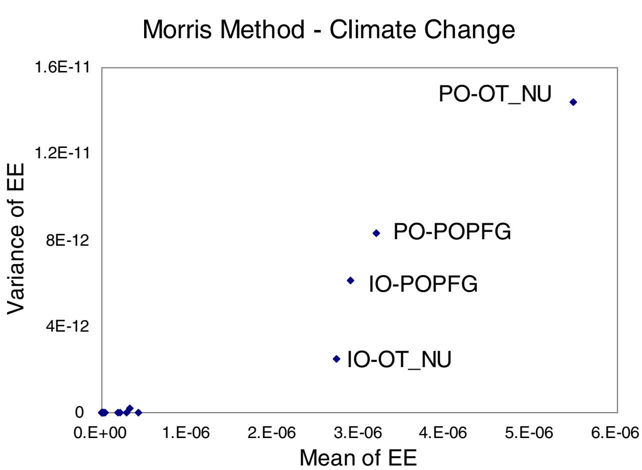

Fig. 4 Morris graph relative to the "Climate change" results for the whole plant model

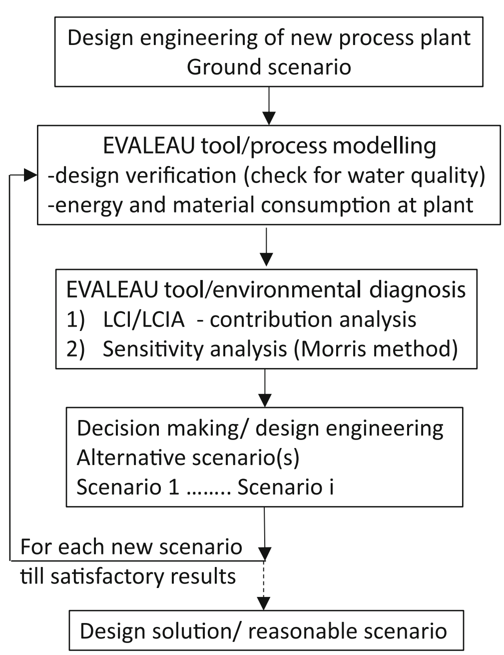

Fig. 5 Use of EVALEAU tool for the eco-design of water treatment processes

production ("POPFG"). So the Morris method indicates that the operation conditions of the two ozonation processes are the main lever actions for improving the plant's environmental performance with respect to the chosen impact category. Both operating parameters intervene in the energy consumption calculation for the ozone production at plant. The improvement of the ozone production technology and of the ozone/water contactor is therefore the main priority action in the aim of decreasing the energy consumption and the related impacts.

4 Conclusions

The concepts and methodologies embedded within the developed PM-LCA tool, named EVALEAU for water treatment, provide the user with complementary views of the designed system. The modelling principle which consists in parameterizing a generic model to get a project-specific model enables the user to cope with high variability of water treatment processes and water quality. The tool allows to address the project constraints and to test the engineering design choices, thus providing useful support to eco-design. Sensitivity analysis of the model parameters suing the Morris method is an original feature of the tool as well and provides a significant added value to plant operators. EVALEAU successfully solved the problem of linking LCA results with the related engineering design choices and operation parameters. To our knowledge, it is the first fully fledged integrated PM-LCA tool for environmental assessment and design of processes, specifically developed and targeted to the water industry.

The EVALEAU tool could be used in an eco-design process (Fig. 5) since it combines two functions: *process modelling-design aid* and *environmental diagnosis*. In the design engineering of a new plant, it can be used for the verification of the initial technological choices ("ground scenario") against the produced water's quality requirements, by using the *process modelling* function of the tool. Then, the *environmental diagnosis* function provides two complementary features: (1) LCIA and contribution analysis and (2) sensitivity analysis on process parameters with respect to the selected impacts. The results supplied by the EVALEAU tool allow therefore identifying and assessing relevant design options ("alternative scenarios"), relative to the replacement of UPs for instance, or to the modification of design and operation parameters, of reactants, etc. The tool shall be consistently applied to all the selected scenarios, for technological verification followed by environmental diagnosis. The eco-design process could be iterated until an optimal solution is found following the chosen criteria (environmental but also economic and technical).

The test bed case presented in this paper uses only part of the UP modules existing in the EVALEAU library, which covers most of the UPs processes based on physicochemical mechanisms, currently used for potable water production and waste water treatment. The application case shows the reliability of the models used for describing the UPs: (1) the plant's model, with appropriate parameter values, is able to reproduce the water quality transformation in the treatment chain, the water being the functional flow, and (2) the PM-LCA tool generates relevant LCI/LCIA results when compared to conventional LCA results.

During the development of the tool, special attention was given to the software architecture, in order to anticipate further developments. The tool has the necessary flexibility to integrate future expert recommendations as well as novel technologies. The user can introduce additional functionalities through the integrated scripting (e.g., integrating optimization algorithm to choose the best set of parameter values). The robustness of the tool also benefits from the linking with external, specialized and well recognized software as PHREEQC® for complex aqueous chemistry modelling.

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